1-Hexadecanol, 5-chloro, acetate

Other names: 5-Chlorohexadecyl acetate
Inchi: InChI=1S/C18H35ClO2/c1-3-4-5-6-7-8-9-10-11-14-18(19)15-12-13-16-21-17(2)20/h18H,
InchiKey: RLIYOHYNGXGNSM-UHFFFAOYSA-N
Formula: C18H35ClO2
SMILES: CCCCCCCCCCCC(Cl)CCCCOC(C)=O
Mol. weight [g/mol]: 318.92

Physical Properties

Property code	Value	Unit	Source
gf	-147.61	kJ/mol	Joback Method
hf	-680.67	kJ/mol	Joback Method
hfus	45.84	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	6.248		Crippen Method
mcvol	284.160	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	2182.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2182.00		NIST Webbook
ripol	2680.00		NIST Webbook
ripol	2691.00		NIST Webbook
ripol	2667.00		NIST Webbook
ripol	2667.00		NIST Webbook
tb	724.52	K	Joback Method
tc	899.87	K	Joback Method
tf	379.70	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.77	J/mol×K	724.52	Joback Method
cpg	843.94	J/mol×K	753.74	Joback Method

cpg	861.23	J/mol×K	782.97	Joback Method
cpg	877.67	J/mol×K	812.19	Joback Method
cpg	893.27	J/mol×K	841.42	Joback Method
cpg	908.06	J/mol×K	870.64	Joback Method
cpg	922.05	J/mol×K	899.87	Joback Method
dvisc	0.0019853	Pa×s	379.70	Joback Method
dvisc	0.0008119	Pa×s	437.17	Joback Method
dvisc	0.0004087	Pa×s	494.64	Joback Method
dvisc	0.0002373	Pa×s	552.11	Joback Method
dvisc	0.0001527	Pa×s	609.58	Joback Method
dvisc	0.0001060	Pa×s	667.05	Joback Method
dvisc	0.0000780	Pa×s	724.52	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R33309&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume